

C:\Documents and Settings\EBernhardt\My Documents\Stnexp\Queries\10550571.str

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ring nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :
    6-16 7-11 16-17 17-18 18-19

ring bonds :
    1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9 10-11 10-15 11-12
    12-13 13-14 14-15

exact/norm bonds :
    1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 6-16 7-8 8-9 16-17

exact bonds :
    7-11 17-18 18-19

normalized bonds :
    10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :
    containing 1 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
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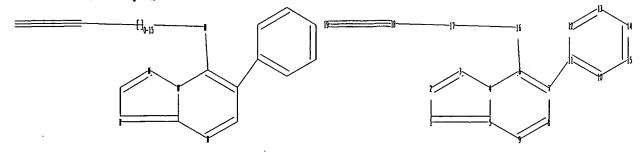
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS

18:CLASS 19:CLASS

17:CLASS

=>

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Documents\Stnexp\Queries\10550571.str



chain nodes : 16 17 18 19 ring nodes: 5 6 7 8 9 10 11 12 13 14 15 chain bonds : 6-16 7-11 16-17 17-18 18-19 ring bonds : 1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 6-16 7-8 8-9 16-17 exact bonds : 7-11 17-18 18-19 normalized bonds : 10-11 10-15 11-12 12-13 13-14 14-15 isolated ring systems: containing 1:

## Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS

## L1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 16:01:26 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 2 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 3\_TO 16

PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 16:01:37 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS 26 ANSWERS

SEARCH TIME: 00.00.01

L3 26 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST ENTRY SESSION 166.94 167.15

SINCE FILE

TOTAL

FILE 'CAPLUS' ENTERED AT 16:01:44 ON 05 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 5 Jul 2006 VOL 145 ISS 2 FILE LAST UPDATED: 4 Jul 2006 (20060704/ED)

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http://www.cas.org/infopolicy.html

=> s 13

L4 3 L3

=> d 14 1-3 bib abs hitstr

L4 (ANSWER 1 OF 3 )CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:857602 CAPLUS

DN 141:332222

TI Methods for the production and use of 7-(alkynylamino)triazolopyrimidines and agents containing them useful for combating harmful fungi

IN Tormo I Blasco, Jordi; Blettner, Carsten; Mueller, Bernd; Gewehr, Markus; Grammenos, Wassilios; Grote, Thomas; Gypser, Andreas; Rheinheimer, Joachim; Schaefer, Peter; Schieweck, Frank; Schwoegler, Anja; Scherer, Maria; Strathmann, Siegfried; Schoefl, Ulrich; Stierl, Reinhard

PA BASF Aktiengesellschaft, Germany

SO PCT Int. Appl., 36 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

	PAT	rent :	NO.			KIN	D	DATE								D	ATE	
PI	WO	2004	0877	06		A1	_	2004	1014			 004-1				2	0040	 330
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		RW:						-	-		SL,			-	_	-	-	
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			TD,	TG		·				•				•	•	•	•	•
		2004				A1					AU 2							
	CA	2520	718		•	AA		2004	1014		CA 2	004-	2520	718		2	0040	330
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	BR	2004	0088	64		Α	•	2006	0411	•	BR 2	004-	8864		•	2	0040	330
		1768									CN 2							
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os		SREAC																
GI																		

AB 7-(Alkynylamino)triazolopyrimidines I [L = halogen, C1-6-alkyl, C1-6-halogenalkyl, C1-6-alkoxy, NH2, NHR, NR2, cyano, S(O)nA1 or C(O)A2; R = C1-8-alkyl, C1-8-alkylcarbonyl; A1 = hydrogen, hydroxy, C1-8-alkyl, C1-8-alkylamino, di(C1-8-alkyl)amino; n = 0, 1 or 2; A2 = C2-8-alkenyl, C1-8-alkoxy, C1-6-halogenalkoxy or A1; m = 1, 2, 3, 4 or 5 (whereby at least one group L is present in an ortho-position to the bond with the triazolopyrimidine skeleton); X = halogen, cyano, C1-4-alkyl, C1-4-haloalkyl, C1-4-alkoxy; R1 = hydrogen, C1-4-alkyl; R2 = (un)substituted C3-10-alkynyl]. The invention also relates to methods for the production of said compds., agents containing said compds. and the use thereof

to combat harmful phytopathogenic fungi. The procedure for the preparation of I is characterized by: reaction of halotriazolopyrimidines II (Hal = halogen) with R1R2NH. Thus, triazolopyrimidine I [R1 = H, R2 = CH2C.tplbond.CH, X = C1, L3 = F3-2,4,6] was prepared from 5,7-Dichloro-6-(2,4,6-trifluorophenyl)[1,2,4]triazolo[1,5-a]pyrimidine (II; ) via amination with HC.tplbond.CCH2NH2 in CH2C12 containing Et3N. The inhibitory activity of I were determined [after 5 d I (R1 = H, R2 = CH2C.tplbond.CCH2C1, X = C1, L3 = F3-2,4,6; R1 = H, R2 = CMe2C.tplbond.CH,

X = Cl, L3 = F3-2,4,6) had decreased the activity of Alternaria solani (Tomato dry spot disease) and Puccinia recondita (wheat brown rust) to 3%].

IT 773879-52-0P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation and nucleophilic substitution reactions of; preparation of (alkynylamino)triazolopyrimidines for use in combating harmful phytopathogenic fungi)

RN 773879-52-0 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-methyl-N-2-propynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

TT 773879-51-9P 773879-53-1P 773879-54-2P 773879-55-3P 773879-56-4P 773879-57-5P 773879-58-6P 773879-59-7P 773879-60-0P 773879-62-2P 773879-63-3P 773879-64-4P 773879-65-5P 773879-66-6P 773879-67-7P 773879-68-8P 773879-69-9P 773879-70-2P 773879-71-3P 773879-72-4P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (alkynylamino)triazolopyrimidines for use in combating harmful phytopathogenic fungi)

RN 773879-51-9 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-2-propynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

F NH- 
$$CH_2$$
-  $C$   $CH$ 

RN 773879-53-1 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-(4-chloro-2-butynyl)-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 773879-54-2 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-(1,1-dimethyl-2-propynyl)-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 773879-55-3 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-6-(2-chloro-6-fluorophenyl)-N-2-propynyl- (9CI) (CA INDEX NAME)

RN 773879-56-4 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-6-(2-chloro-6-fluorophenyl)-N-(1,1-dimethyl-2-propynyl)- (9CI) (CA INDEX NAME)

RN 773879-57-5 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N-2-butynyl-5-chloro-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 773879-58-6 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-(1-methyl-2-propynyl)-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

$$F \qquad F \qquad NH-CH-C \Longrightarrow CH$$

$$F \qquad NN \qquad N \qquad N$$

RN 773879-59-7 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-(1-methyl-2-butynyl)-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 773879-60-0 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-2-pentynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

F NH-CH<sub>2</sub>-C 
$$=$$
 C-Et

RN 773879-62-2 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-(1-methyl-2-pentynyl)-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 773879-63-3 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N-3-butynyl-5-chloro-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

F NH-CH<sub>2</sub>-CH<sub>2</sub>-C
$$\equiv$$
CH

RN 773879-64-4 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-(1-methyl-3-butynyl)-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

$$F \xrightarrow{F} NH - CH - CH_2 - C = CH$$

$$F \xrightarrow{N} N$$

RN 773879-65-5 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-3-pentynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

F NH- 
$$CH_2$$
-  $CH_2$ -  $C$   $C$  -  $Me$ 

RN 773879-66-6 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-4-pentynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 773879-67-7 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-6-(4-fluoro-2-methylphenyl)-N-(1-methyl-2-propynyl)- (9CI) (CA INDEX NAME)

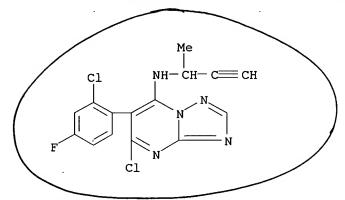
RN 773879-68-8 CAPLUS

## 10/550571

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-6-(2,4-difluorophenyl)-N-(1-methyl-2-propynyl)- (9CI) (CA INDEX NAME)

RN 773879-69-9 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-6-(2-chloro-4-fluorophenyl)-N-(1-methyl-2-propynyl)- (9CI) (CA INDEX NAME)



RN 773879-70-2 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-5-carbonitrile, 7-(methyl-2-propynylamino)-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 773879-71-3 CAPLUS

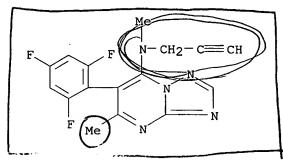
CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-methoxy-N-methyl-N-2-propynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

F Me N- 
$$CH_2$$
-  $C \equiv CH$ 

F MeO N

RN 773879-72-4 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,5-dimethyl-N-2-propynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:77777 CAPLUS

DN 139:292263

TI Preparation of (amino)(aryl)triazolopyrimidines as microbicides

IN Boie, Christiane; Dunkel, Ralf; Elbe, Hans-Ludwig; Gayer, Herbert; Gebauer, Olaf; Krueger, Bernd-Wieland; Heinemann, Ulrich; Voerste, Arnd; Guth, Oliver; Ebbert, Ronald; Wachendorff-Neumann, Ulrike; Mauler-Machnik, Astrid

PA Bayer CropScience AG, Germany; et al.

SO PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

ran. Cni i																		
	PAT	ENT I	NO.			KIN	D	DATE		1	APPL:	ICAT:	ION I	NO.		D	ATE	
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PI	WO	2003	0806	14 <b>°</b>		A2		2003		1	WO 2	003-1	EP24	13	(	(2)	0030:	310 /
	WO 2003080614				<b>A3</b>		20040108											
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     WO 2003-EP2413
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os
     MARPAT 139:292263
GΙ
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AΒ Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, alkenyloxy, alkynyloxy, cycloalkyloxy, (di)alkylamino, alkenylamino, alkynylamino, cycloalkylamino, N-cycloalkyl-N-alkylamino, alkylidenamino, heterocyclyl; R2 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; NR1R2 = (substituted) heterocyclyl; R3 = (substituted) aryl; R4 = halo, cyano, (substituted) alkoxy or dialkylamino; X = halo, were prepared Thus, 2,5,7-trichloro-6-(2chlorophenyl)-1,2,4-triazolo[1,5-a]pyrimidine (preparation given) in CH2Cl2 was treated with isopropylamine and Et3N followed by stirring for 2 h at 60° to give 18% N-[2,5-dichloro-6-(2-chlorophenyl)-1,2,4triazolo[1,5-a]pyrimidin-7-yl]-N-isopropylamine. Several I at 100-199 ppm gave 83-100% control of Podosphaera leucotricha on apple. IT 608089-38-9P RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN

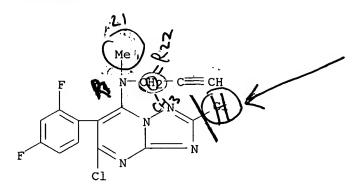
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (amino)(aryl)triazolopyrimidines as microbicides) 608089-38-9 CAPLUS

[1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 2,5-dichloro-6-(2,4-difluorophenyl)-N-methyl-N-2-propynyl- (9CI) (CA INDEX NAME)

RN

CN



L4ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN ΑN 2002:849630 CAPLUS 137:353057 DN ΤI Preparation of 1,2,4-triazolo[1,5-a]pyrimidines as agricultural bactericides and fungicides IN Gebauer, Olaf; Greul, Joerg Nico; Heinemann, Ulrich; Elbe, Hans-Ludwig; Krueger, Bernd-Wieland; Dunkel, Ralf; Voerste, Arnd; Ebbert, Ronald; Wachendorff-Neumann, Ulrike; Kuck, Karl-Heinz; Kitagawa, Yoshinori PΑ Bayer Aktiengesellschaft, Germany SO PCT Int. Appl., 112 pp. CODEN: PIXXD2 DTPatent German LА FAN.CNT 1

LWIN.	CNII					
	PATENT NO.		APPLICATION NO.	DATE		
PΙ	WO 2002088127	A2 20021107	WO 2002-EP4441	20020423		
	WO 2002088127	A3 20021227				
	W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, BZ,	CA, CH, CN,		
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	DE 10121102	A1 20021107	DE 2001-10121102	20010427		
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os	MARPAT 137:353057					

GI

$$NR^{1}R^{2}$$
 $N^{1}R^{2}$ 
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 $N^{1}R^{2}$ 
 $N^{1}R^{2}$ 

Title compds. [I; R1 = amino, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, alkenyloxy, alkynyloxy, cycloalkoxy, alkylamino, dialkylamino, alkenylamino, alkynylamino, cycloalkylamino, N-cycloalkyl-N-alkylamino, alkylideneamino, heterocyclyl, SR5; R5 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; or NR1R2 = heterocyclyl; R3 = (substituted) aryl; R4 = (substituted) alkyl, alkenyl, alkynyl; X = halo; n = 0-2] and salts thereof were prepared Thus, a mixture of 5,7-dichloro-2-(methylsulfanyl)-6-(2,4,6-trifluorophenyl)-1,2,4-triazolo[1,5-a]pyrimidine (preparation given) and 4-trifluoromethylpiperidine in CH2Cl2 was treated with Et3N followed by stirring for 18 h at room temperature to give 83.4% 5-chloro-7-[4-(trifluoromethyl)-1-piperidinyl]-6-(2,4,6-trifluorophenyl)-1,2,4-triazolo[1,5-a]pyrimidine. Several I at 100 ppm gave 94-100% control of Podosphaera leucotricha.

IT 474507-44-3P 474508-09-3P 474509-00-7P 474509-93-8P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of triazolopyrimidines as agricultural bactericides and fungicides)

RN 474507-44-3 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-methyl-2-(methylthio)-N-2-propynyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

RN 474508-09-3 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-6-(2,6-difluorophenyl)-N-methyl-2-(methylthio)-N-2-propynyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
Me \\
N-CH_2-C \longrightarrow CH \\
N & SMe
\end{array}$$

RN 474509-00-7 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-N-methyl-2-(methylthio)-6-(pentafluorophenyl)-N-2-propynyl- (9CI) (CA INDEX NAME)

$$F \qquad F \qquad N - CH_2 - C = CH$$

$$F \qquad N \qquad N \qquad SMe$$

$$F \qquad C1 \qquad N \qquad N$$

RN 474509-93-8 CAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 5-chloro-6-(2,4-difluorophenyl)-N-methyl-2-(methylthio)-N-2-propynyl- (9CI) (CA INDEX NAME)

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